
# SESSION: COMPUTATIONAL PHYSICS, COMPUTATIONAL FLUID DYNAMICS, AND SOLID MECHANICS (PFD)

# INVITED SPEAKERS

## PFD-I-01
## Molecular Simulations of Bio-Interfaces for Sensor Development

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### ABSTRACT

***Keywords**: molecular simulations, graphene, gold, aptamers, biomolecules, sensors*

The interface between biomolecules and solid surfaces or nanoparticles is relevant to a range of defence areas including photonics and plasmonics, energy generation and harvesting, armour and protection, and biosensing.[1] To drive these applications forward, we need to understand how to manipulate the structures of these biomolecules adsorbed at the nano-interface. In partnership with experimental characterization, molecular simulations (Figure 1) can bring unique insights into these interfacial structures.[2] Our team specialise in the development and deployment of advanced molecular simulation techniques for these purposes. Here, I will summarize our collaborative developments with experimental researchers[3] to determine structure/property relationships of these interfaces.

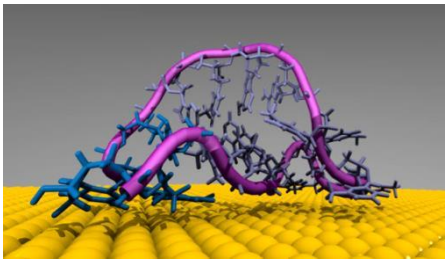

**Figure 1.** Snapshot taken from a molecular dynamics simulation of a DNA hairpin adsorbed on the Au(111) surface (water not shown).

### REFERENCES

1. T. R. Walsh and M. R. Knecht, *Chem. Rev.*, 2017, 117, 12641-12704

T. R. Walsh, *Acc. Chem. Res.*, 2017, 50, 1617-1624.

Martin, J. A.; Chavez, J. L.; Chushak, Y.; Chapleau, R. R.; Hagen, J.; Kelley-Loughnane, N., Anal Bioanal Chem 2014, 406 (19), 4637-4647.

**PFD-I-01**

**Tiffany Walsh** earned her PhD degree from University of Cambridge. She held a Glasstone Fellowship in Dept of Materials at the University of Oxford, and joined the Dept. of Chemistry, University of Warwick. She is a Professor of Bio/Nanotechnology at the Institute for Frontier Materials, Deakin University. Her research interests focus on computational modelling the interface between soft matter and synthetic materials.

# PFD-I-02
# Molecular Dynamics Simulations of the Self-Sssembly of Drug-Delivery Vehicles

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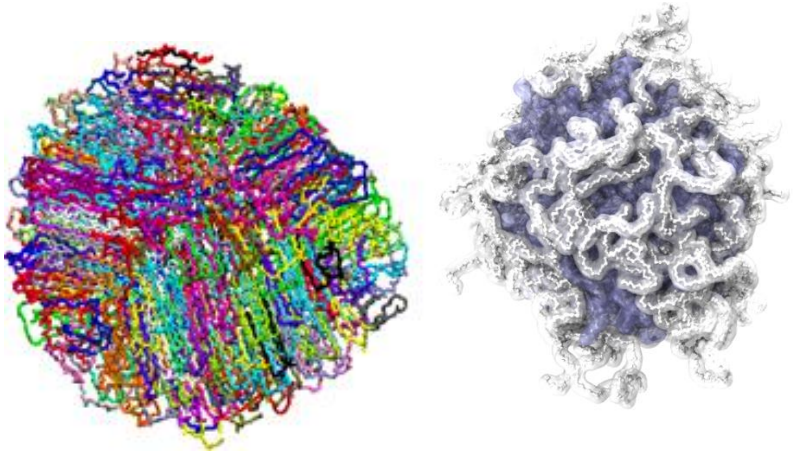
## ABSTRACT

***Keywords**: Molecular dynamics, polymers, lipids, drug-delivery, self-assembly*

Nanomedicine has continuously been in the spotlight according to the immense popularity of nanoscience and nanotechnology. Engineered nanomaterials have been specifically designed for various applications, including drug delivery, biomedical imaging, bio-sensing, diagnostics and therapy. Both polymer- and lipid-based nanoparticles have received intensive attention in the area of drug delivery systems because the hydrophobic drug molecules can be encapsulated in these self-assembled nanoparticles. In order to optimise the design of these drug-delivery vehicles, knowledge of the interactions that govern their self-assembly and the encapsulation of small molecules. Molecular dynamics simulations are frequently used as a tool to gain insight into the molecular scale interactions that govern the behaviour of materials of all types. In this talk, I will present the recent work done in my group in which we have used molecular dynamics simulations to investigate solid-lipid nanoparticles and polymeric nanoparticles. In both cases, I will demonstrate how we have used our simulations alongside complimentary experimental methods to provide as detailed a multi-scale picture of these systems as possible.



**PFD-I-02**

**Chris Lorenz** got his PhD in Chemical Engineering from the University of Michigan (2001). Currently he is a Professor in Physics in the Biological Physics and Soft Matter Group in the Department of Physics, King's College London. His research interests focus on the application of molecular dynamics simulations to investigations of a variety of problems in the areas of soft-matter self-assembly and biophysics.

# PFD-I-03

# Molecular Simulations from Physicists' Point of View: Applications for Biosensors, Polymers, and Proteins

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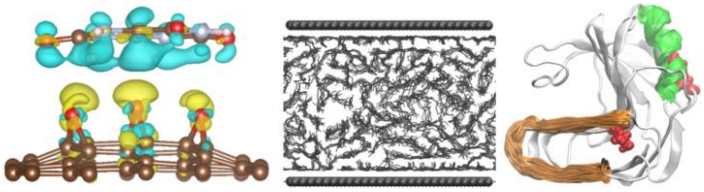
## ABSTRACT

***Keywords**: Molecular Simulations, Biosensors, Protein Engineering*

This talk presents basic principles of molecular simulation techniques and some previous examples of visualizing molecular systems in atomistic details that help solving some challenge problems in biosensing, polymers, and protein engineering. Firstly, fundamental of electrochemical selectivity enhancement for ascorbic acid (AA), dopamine (DA), and uric acid (UA) was unveiled both by density functional theory (DFT) calculations and atomistic molecular dynamics (MD) simulations [1]. The simultaneous detection of the AA/DA/UA system has been an open problems in the field of biosensing. Then, another problem on the local glass transition of polymers induced by carbon-based fillers was investigated. A microscopic point of view on the molecular motion led to the total understanding of local transition from the 'rubbery' into the 'glassy' regime and the connection between microscopic and the macroscopic worlds [2]. Finally, two applications on protein engineering are mentioned: (1) two single-point mutations led to a synergistic effect that enhance the protein stability [3] and (2) the mechanisms of how protonation of lysozymes at low pH induced the formation of beta structures was also clarified [4].



## REFERENCES

1. Prasert, K.; Sutthibutpong, T. PHYSICAL SCIENCES, 2021.
2. Sutthibutpong, T. Modelling Simul. Mater. Sci. Eng. 2021, 29, 045002, doi:10.1088/1361-651X/abdc6d.
3. 3Boonyaputthikul, H.; Muhammad, A.; Roekring, S.; Rattanarojpong, T.; Khunrae, P.; Sutthibutpong, T. Archives of Biochemistry and Biophysics 2019, 672, 108068, doi:10.1016/j.abb.2019.108068.
4. Zein, H.F.; Alam, I.; Asanithi, P.; Sutthibutpong, T. Biophysics, 2021.

***PFD-I-03***

**Thana Sutthibutpong** received his PhD degree from the University of Leeds in 2015. Currently he is a Asst Prof in the Department of Physics, KMUTT. His research interests focus on applying molecular simulation techniques to explain molecular mechanisms underlying biomolecules and materials..

# ORAL PRESENTATION

## PFD-O-01

# A computational Fluid Dynamics (CFD) study on coke formation behavior over a spherical alumina-supported nickel catalyst ($Ni/Al_2O_3$) particle for dry reforming of methane

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## ABSTRACT

***Keywords***: *CFD, Dry reforming of methane, Coke formation*

Dry reforming of methane (DRM), the solid-catalyzed gas-phase reaction can convert greenhouse gases into synthetic gas. However, the coke formation over the catalyst particle is a major problem, which will lead to catalyst deactivation. In this work, the three-dimensional (3D) computational fluid dynamics (CFD) simulation with chemical reactions which was performed by commercial software ANSYS Fluent to investigate coke formation behaviour over a spherical alumina-supported nickel catalyst ($Ni/Al_2O_3$) particle. A single spherical catalyst particle model was used with a particle diameter of 2 mm and pore diameter of 10 nm. The $CH_4/CO_2$ molar ratio of unity was used. The distribution of temperature, reactant and product profiles inside the catalyst particle were also analyzed. The results show good agreements with experimental data. In addition, the difference of coke accumulation between catalyst surface and within the particle zone was observed.

## REFERENCES

1. J. Richardson, S. Paripatyadar, Applied Catalysis 1990, 61, 293-309.
2. J.-W. Snoeck, G. Froment, M. Fowles, Journal of Catalysis 1997, 169, 250-262.
3. J.-W. Snoeck, G. Froment, M. Fowles, Industrial & engineering chemistry research 2002, 41, 4252-4265.
4. X. Yang, S. Wang, K. Zhang, Y. He, Chemical Engineering Science 2021, 229, 116122.
5. E. L. Lugo, B. A. Wilhite, Chemical Engineering Science 2016, 150, 1-15.
6. Z. Hou, P. Chen, H. Fang, X. Zheng, T. Yashima, International journal of hydrogen energy 2006, 31, 555-561.
7. Al-Fatesh, Journal of King Saud University-Engineering Sciences 2015, 27, 101-107.
8. G. Karthik, V. V. Buwa, Reaction Chemistry & Engineering 2020, 5, 163-182.

# PFD-O-02

# Study of Heat and Mass Transfer in MHD Flow of Sutterby Nanofluid over a Curved Stretching Sheet with Magnetic dipole and effect

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## ABSTRACT

***Keywords***: *Chemical reactions, Curved surface, Heat transfer, Magnetic dipole, Thermal radiation, Sutterby ferrofluid*

A systematic study of non-Newtonian Sutterby ferrofluid and heat transfer in the flow due to curved stretching sheets is presented. Flow is caused by the linear velocity of the curved sheet. Concentration and energy equations are incorporated in the study of mass and heat transfer impacts. The motile microorganism equation included the swimming of the gyrotactic microorganism. The governing equations are transformed from partial differential equation to ordinary differential equation and the solved using Homotopy Analysis method. The velocity is reduced due to dipole and non-Newtonian parameters effects. Temperature increases with the dipole effect and thermal radiation parameters. Concentration decreases with an increase in the homogeneous chemical reaction parameter and the concentration of microorganisms decreases with the Lewis number. Streamlines show that trapping on the curved stretched surface is uniform.

## REFERENCES

1. Liao, S.J. The proposed homotopy analysis method for the solution of nonlinear problems. Ph.D. Thesis, *Shanghai Jiao Tong University, Shanghai, China* **1992**.
2. Sudhagar, P.; Kameswaran, P.K.; Kumar, B.R. Gyrotactic microorganism effects on mixed convective nanofluid flow past a vertical cylinder. *J. Therm. Sci. Eng. Appl.* **2019**, *11*.
3. Sutterby JL. Laminar converging flow of dilute polymer solutions in conical sections. II. *Transactions of the Society of Rheology*. 1965 Sep;9(2):227-41.
4. Andersson HI, Valnes OA. Flow of a heated ferrofluid over a stretching sheet in the presence of a magnetic dipole. *Acta Mechanica*. 1998; 128: 39-47.

# PFD-O-03

# Biomechanical evaluation of screw configurations on conventional plate fixation in humeral shaft fracture using finite element analysis

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## ABSTRACT

***Keywords***: *Humeral shaft fracture, Plate and screw fixation, Screw configurations, Finite element analysis*

A standard technique of humeral shaft fracture treatment is plate and screw fixation .Bicortical screws are commonly used in this technique .However, previous studies reported that the tip of bicortical screws could damage radial nerve .To avoid the nerve injury, this study was evaluated the biomechanical properties and optimized the appropriate condition of screw configurations in the humeral shaft fracture using finite element analysis .Simple humerus models were allocated into six different screw length configurations .All models were tested in axial compression, torsion, and bending .The construct stability was investigated by stiffness, relative displacement, and von Mises stress .The non-inserted screw at the risk position of radial injury provided low stability which considered by the lowest stiffness in torsion, the highest relative displacement in torsion and bending, and the lowest von Mises stress compared to other configurations .At the risk position, there was no significant difference in bicortical, unicortical and unicortical abutting screw . These results suggested that the replacement of unicortical and unicortical abutting screw at the risk position could provide stability equivalent to bicortical screw fixation .Therefore, this finding may suggest the screw configurations to remove the risk of radial nerve injury .

## REFERENCES

1. Apivatthakakul T, Patiyasikan S, Luevitoonvechkit S ,.*et al., Injury*, 2009 ,**41** ,169-72.
2. Antoniac I, Stoia D, Ghiban B, Tecu C, Miculescu F, Vigaru C., et al ,.*Materials*, 2019 ,**12** ,1128.
3. Croley J, Morris R, Amin A, Lindsey R, Gugala Z ,.*et al., The journal of hand surgery,* 2016, **41**

# PFD-O-04

# Biomechanical evaluation of four fixation methods in two-tunnel Coracoclavicular ligament reconstruction technique using Finite element analysis

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## ABSTRACT

***Keywords***: *AC joint dislocation, CC reconstruction, Evaluation of AC joint treatment, Finite element analysis*

To treat Acromioclavicular (AC) joint dislocation, the two-tunnel Coracoclavicular (CC) ligaments reconstruction technique is a recommended technique. However, there presents failures from this technique including tunnel widening and loss of reduction. Previous studies found that the multiple choice of fixation types may affect treatment failure. Therefore, this study aimed to investigate the stability and effect of four different fixation methods in two-tunnel CC ligament reconstruction technique using Finite element analysis (FEA). The simplified surgical procedures were created in four models, which different in tunnel positions and fixation methods. All models were applied 70 N load in three directions. Maximum von Mises stress and displacement were analysed. The maximum stress of clavicle bone in all models provided lower value than bone yield strength (114 MPa). Interestingly, perpendicular tunnel position with O-loop fixation generated lower stress value in all direction tests than other models. This fixation also exhibited the lowest displacement value in superior direction, which represented a good stability. Perpendicular tunnel position with O-loop fixation method may help to decrease risk of failure after treatment due to cumulative stress in the construct.

## REFERENCES

1. Çalışal E, Uğur L, *Acta Orthop Traumatol Turc.* 2020, **54** (2), 202-6.
2. Weiser L, Nüchtern JV, Sellenschloh K, Püschel K, Morlock MM, Rueger JM, et al., *Knee Surgery, Sports Traumatology, Arthroscopy*, 2017, **25** (7), 2025-31.
3. Clavert P, Meyer A, Boyer P, Gastaud O, Barth J, Duparc F, *Orthopaedics & Traumatology: Surgery & Research*, 2015, **101** (8), S313-S6.
4. Kennedy BP, Rosenberg ZS, Alaia MJ, Samim M, Alaia EF, *Skeletal Radiology*, 2020, **21** (1432-2161), 1-11.

# PFD-O-05

# *In silico* study of signature interactions between methylated DNA and graphene oxide nanosheet for universal cancer screening

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## ABSTRACT

***Keywords:*** *Graphene oxide nanosheet; Methylated DNA; Molecular dynamics (MD) simulation; Density functional theory (DFT)*

DNA methylation, an epigenetic process by which methyl groups are added to DNA, is associated with carcinogenesis. It could serve as a universal cancer biomarker [1]. Therefore, signature interactions between methylated DNA and nanomaterials such as graphene oxide (GO) can pave the way for DNA methylation detection. To unveil their macro- and micro-level mechanisms, molecular dynamics (MD) simulation and density functional theory (DFT) have been conducted. According to the MD simulations, methylated and unmethylated DNAs were adsorbed onto GO with different contacting surface areas (CSAs). The CSA of the methylated and unmethylated ssDNA in water were ~13 $nm^2$ and ~5 $nm^2$, respectively, indicating that GO was more favourable for adsorption of methylated DNA. In the presence of divalent ions ($Mg^{2+}$), the CSA of both cases was ~8 $nm^2$, suggesting that different adsorption can be observed in water. Based upon DFT calculation, energy gap of pristine graphene (*p*G) and GO in the presence of 5-methylcytosine (5mC) were 1.6 and 12.9 meV, respectively, while the adsorption of cytosine resulted in lower energy gap (1.2 meV for *p*G and 9.5 meV for GO). The results in different electrical conductivity of GO will open the door for universal cancer screening approaches based on GO.

## REFERENCES

1. Sina, Abu Ali Ibn, *et al.*, *Nat. commun.*, 2018, **9**(1), 1-13.

# PFD-O-06

# A molecular dynamics study on the diffusion and imprint ability of spectinomycin under different sizes of aniline oligomers

**Chanadan Douykhumklaw[1,2], Ibra Alam[1], Piyapong Asanithi[1], and Thana Sutthibutpong[1,2*]**

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## ABSTRACT

***Keywords**: Molecular dynamics simulation, Molecularly imprinted polymer, Aniline, Spectinomycin*

Molecularly imprinted polymer (MIP) is the polymer created by molecular imprinting techniques that leaves cavity for the specific interactions with a template molecule, and has been applied in molecular selectivity tasks. In this study, molecular dynamics (MD) simulation was used to prove that aniline oligomer could be developed as an MIP for the detection and separation of the spectinomycin drug molecule for gonorrhoea treatment. MD simulations were performed to compare the mean square displacement (MSD) and the diffusivity of spectinomycin within aniline oligomers of different sizes. The calculations showed that the diffusion coefficient was significantly dropped when the size of aniline oligomer is more than two monomers. Then, the distances between pairs of aniline monomers were measured to monitor the geometry of cavity created when the spectinomycin is absent. The analysis showed that aniline tetramer sustained most of its cavity geometry and therefore the optimal oligomer size for further development of MIP.

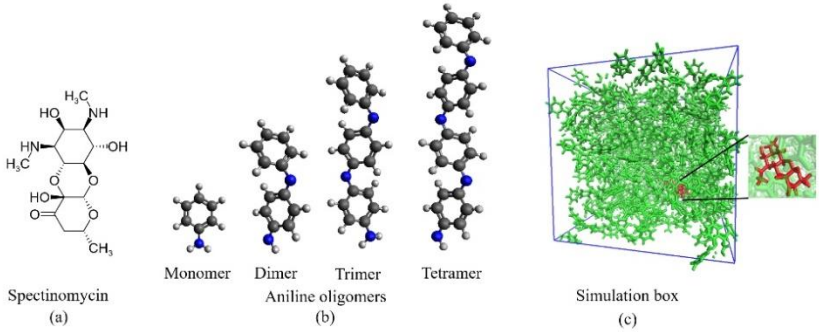


**Figure 1**. Chemical structures and simulation setup for proved by MD; (a) spectinomycin that is template molecule; (b) aniline oligomer; and (c) 64 $nm^3$ simulation box that was added spectinomycin and anilines

## REFERENCES

1. D. Luo, Z. Zhao, *et al*, *Molecular Simulation*, 2014, **40**(6), 431-438.
2. Z. Zhao, Q. Wang, *et al.*, *J. Phys. Chem. B*, 2008, **112**(25), 7515-7521.
3. G. Bagdžiūnas, *Mol. Syst. Des. Eng,* 2020, **5**, 1504-1512.

# PFD-O-07
# An exact analysis of unsteady MHD free convection flow of some nanofluids accounting heat radiation and injection/consumption

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## ABSTRACT

***Keywords:*** *MHD, Laplace transform, Porous material, Nanofluid*

This article investigates the influence of ramped wall velocity and ramped wall temperature on time dependent, magnetohydrodynamic (MHD) natural convection flow of some nanofluids close to an infinitely long vertical plate nested in porous medium. Combination of water as base fluid and three types of nanoparticles named as copper, titanium dioxide and aluminum oxide is taken into account. Impacts of nonlinear thermal radiation flux and heat injection/consumption are also evaluated. The solutions of principal equations of mass and heat transfer are computed in close form by applying Laplace transform. The physical features of connected parameters are discussed and elucidated with the assistance of graphs. The expressions for Nusselt number and skin friction are also calculated and control of pertinent parameters on both phenomena is presented in tables.

## REFERENCES

1. S.U.S. Choi, J.A. Eastman, Enhancing thermal conductivity of fluids with nanoparticles. Technical report, Argonne National Lab., IL (United States), 1995.
2. R.L. Hamilton, O.K. Crosser, Thermal conductivity of heterogeneous two-component systems. Industrial & Engineering Chemistry Fundamentals 1(3), 187–191, 1962.

# PFD-O-08
# Unsteady Radiative Natural Convective MHD Nanofluid Flow Past a Porous Moving Vertical Plate with Heat Source/Sink

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## ABSTRACT

***Keywords:*** *MHD, Volume fraction, Thermal radiation, Nanofluid*

In this research article, we investigated a comprehensive analysis of time-dependent free convection electrically and thermally conducted water-based nanofluid flow containing Copper and Titanium dioxide (Cu and TiO2) past a moving porous vertical plate. A uniform transverse magnetic field is imposed perpendicular to the flow direction. Thermal radiation and heat sink terms are included in the energy equation. The governing equations of this flow consist of partial differential equations along with some initial and boundary conditions. The solution method of these flow interpreting equations comprised of two parts. Firstly, principal equations of flow are symmetrically transformed to a set of nonlinear coupled dimensionless partial differential equations using convenient dimensionless parameters. Secondly, the Laplace transformation technique is applied to those non-dimensional equations to get the close form exact solutions. The control of momentum and heat profile with respect to different associated parameters is analyzed thoroughly with the help of graphs.

## REFERENCES

1. S.U.S. Choi, J.A. Eastman, Enhancing thermal conductivity of fluids with nanoparticles. Technical report, Argonne National Lab., IL (United States), 1995.
2. R.L. Hamilton, O.K. Crosser, Thermal conductivity of heterogeneous two-component systems. Industrial & Engineering Chemistry Fundamentals 1(3), 187–191, 1962.

# PFD-O-09
# Grid Spacing for Efficient Data Center CFD Simulation: A Preliminary Study

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## ABSTRACT

***Keywords:*** *CFD, Data Center, Grid Spacing, Non-conformal Grid*

With increasing power densities in next-generation data center equipment, Computational Fluid Dynamics (CFD) is a promising tool for identifying cooling inefficiencies to save costs and improve server reliability [1]. The accuracy of these simulations depends on grid spacing. While fine grids capture flow characteristics more accurately, their heavy computational demands render them impractical in large-scale simulations. Therefore, determining suitable grid spacing is the key to balancing simulation accuracy and computational demands [2].

In this preliminary work, we explored the extent of simulation accuracy which gains from grid refinement. Here, we investigated the effect of grid spacing on data center simulation results using a steady-state pressure-based SIMPLEC solver. To determine the effect of the proposed method, we performed two near-constant refinements on a uniform grid and assessed spatial convergence with Roache's Grid Convergence Index [3]. The relative errors of each grid were calculated based on values obtained by Richardson extrapolation [4]. A non-conformal grid was created with spacing informed by the uniform grid error data.

Our preliminary results suggest that uniform, locally-coarsened non-conformal grids produce results comparable to conformal grids with similar minimum spacing. A further study would involve assessing potential efficiency gains from non-uniform grids by performing unidirectional coarsening.

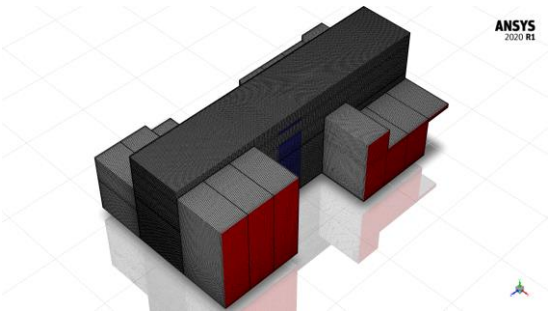


**Figure 1**. Non-conformal cold-aisle data center grid with localized refinement.

## REFERENCES

1. J. Judge, J. Pouchet, S. Dixit, ASHRAE Journal, 2008, 50(11), 14-26.
2. J.W .VanGilder and X .Zhang, ASHRAE Transactions, 2008, 114, 166-181.
3. P .J .Roache, J .Fluids Eng., 1994, 116)3(, 405-413.
4. P. J. Roache, Annu. Rev. Fluid. Mech., 1997, 29, 123–160.

# POSTER PRESENTATION

## PFD-P-01

## Extremely localized basis functions for band structure calculations and an approximated case: Finite difference approximation

**Pairot Moontragoon[1,2,3,*], Natdanai Namwong[1], Vittaya Amornkitbamrung[3], Santi Maensiri[4], and Zoran Ikonic[5]**

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### ABSTRACT

***Keywords***: *Dirac delta function, basis function, variational method, group IV semiconductors*

In this work the Dirac delta comb function is used as a basis function to approximate the full wave function in the variational method. The validity of using this basis function was tested by calculating the electronic band structure of silicon (Si), germanium (Ge) and α-tin (Sn) in diamond structure (having 8 atoms in cubic unit cell), using the modified Falicov type of atomic formfunctions. The kinetic energy term of the Hamiltonian was approximated by the second order central finite difference method, which makes the Hamiltonian matrix identical to that obtained by conventional finite difference method, which shows the identity of the two approaches. The computation time per one k-point in the band structure diagram by using 3024 basis functions with the Dirac delta function basis is smaller than with the plane waves basis, e.g. requiring 0.293, 0.206 and 0.28 minutes for the full band structure when using finite difference approximations with the order of accuracy of $\Delta^2$, $\Delta^4$, and $\Delta^6$, respectively, compared to 0.48 minutes with the plane wave basis, which is widely used in electronic structure codes, making the $\Delta^4$ finite difference accuracy with the Dirac delta basis the most efficient choice. Furthermore, the Dirac delta function basis shows their method with scales as O(n), while the plane wave approach should scale as O(n log n) and with the complexity of the fast Fourier transform.

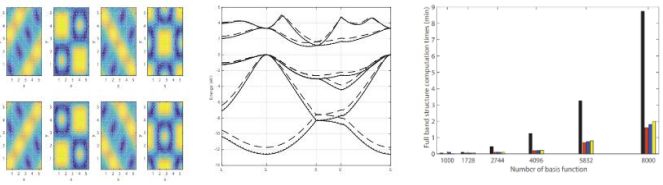

**Figure 1**. (Top left) The potential in real space in silicon unit cell, (Top right) the energy band structure of silicon calculated with plane waves basis (solid), and with the Dirac delta functions basis with the finite difference approximation, and (bottom) the full energy band structure computation time, calculated with the plane waves basis (black) and with the Dirac delta functions basis with the finite difference approximation.

### REFERENCES

1. R. Thirayatorn, P. Moontragoon, V. Amornkitbamrung, S. Meansiri, Z. Ikonic, "Finite-difference calculation of the electronic structure of artificial graphene, the 2D hexagonal $Al_wGa_{1-w}As$/GaAs structure with tunable interactions", Computer Physics Communications, 2015, 191, 106-118.